

# The sign problem in Lattice QCD

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# Scope of lattice QCD simulations: Physics of color singlets

- \* “One-body” physics: confinement  
hadron masses  
form factors, etc..

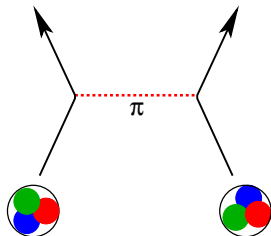


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pioneers Hatsuda et al, Savage et al



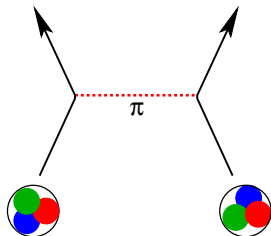
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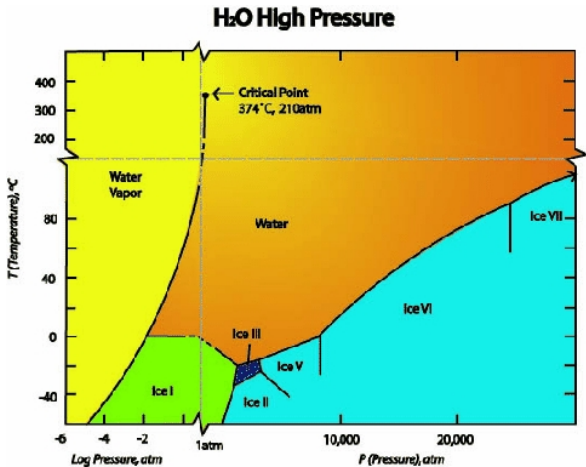
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hard-core  
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- \*\*\* Many-[composite]-body physics: nuclear matter  
phase diagram vs (temperature  $T$ , density  $\leftrightarrow \mu_B$ )

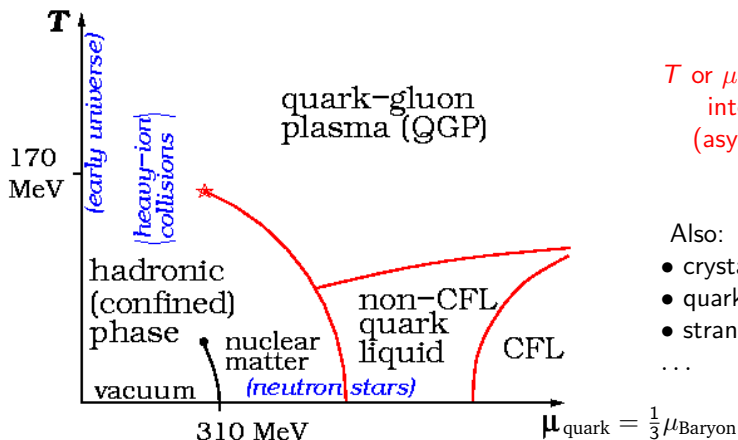
Water changes its state when heated or compressed



What happens to quarks and gluons when heated or compressed?

# The phase diagram of QCD according to Wikipedia

## Current conjecture



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

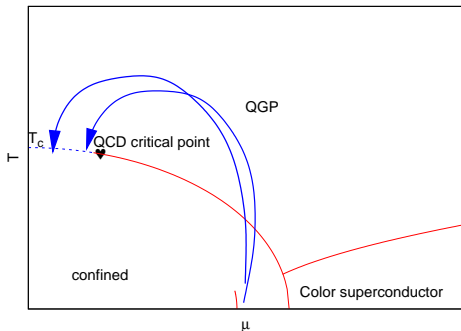
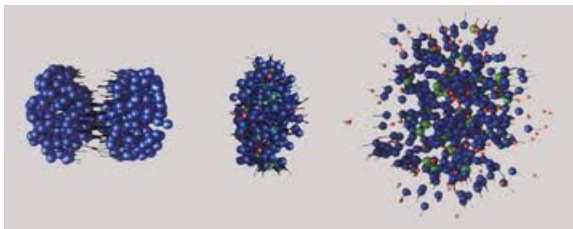
Also:

- crystal phase(s)
- quarkyonic phase
- strangelets
- ...

A vast world to explore and map out!

A "race" between experiment (heavy-ion collisions) & theory (lattice QCD)

# 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)

# Lattice QCD

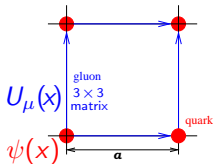
Degrees of freedom at each Euclidean time:

positions of  $N$  particles  $(x_1, x_2, \dots, x_N)$   $\longrightarrow$  *field*  $\phi(x)$



# Lattice QCD

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



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

- Discretized action  $S_E$ :

- $\rightarrow \bar{\psi}(x) U_\mu(x) \psi(x + \hat{\mu}) + h.c.,$

Dirac operator  
 $\bar{\psi} \mathcal{D} \psi$

- $\rightarrow \beta \text{ReTr} U_P, U_P \text{ plaquette matrix}$



Yang-Mills action  
 $\frac{1}{4} F_{\mu\nu} F_{\mu\nu}$

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

$$\text{Prob}(\text{config}\{U\}) \propto \det^2 \mathcal{D}(\{U\}) e^{+\beta \sum_P \text{ReTr} U_P} \text{ real non-negative when } \mu = 0$$

# Lattice QCD Monte Carlo: sources of errors

- **Systematic** errors:

$$\left\{ \begin{array}{l} L \rightarrow \infty, \text{ thermodynamic limit} \\ a \rightarrow 0, \text{ continuum limit} \\ m_q \searrow m_{\text{phys}} \end{array} \right.$$

Extrapolations guided by analytic ansätze (asymptotic freedom,  $\chi$ PT)

- **Statistical** (Monte Carlo) errors:  $\propto 1/\sqrt{\#\text{configs}}$ .

30 years of steady progress since **Mike Creutz, 1980**:

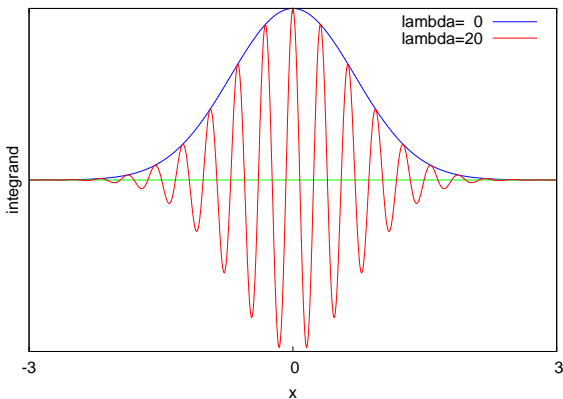
Both errors have been shrinking thanks to **hardware** + **algorithmic** progress

→ Universal tool for **static, equilibrium** properties of QFT



# Sampling oscillatory integrands

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



- $Z(\lambda)/Z(0) = \exp(-\lambda^2/4)$ : exponential cancellations  
→ truncating deep in the tail at  $x \sim \lambda$  gives  $\mathcal{O}(100\%)$  error  
“Every  $x$  is important” ↔ How to sample?

# Reweighting and optimal sampling of oscillatory integrand

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

Sample w.r.t. **auxiliary partition function**  $Z_g \equiv \int dx g(x)$ ,  $g(x) \geq 0 \forall x$

$$\langle W \rangle_f \equiv \frac{\int dx W(x) f(x)}{\int dx f(x)} = \frac{\frac{1}{Z_g} \int dx W(x) \frac{f(x)}{g(x)} g(x)}{\frac{1}{Z_g} \int dx \frac{f(x)}{g(x)} g(x)} = \frac{\langle W \frac{f}{g} \rangle_g}{\langle \frac{f}{g} \rangle_g} \quad \frac{f}{g} \text{ is "reweighting factor"}$$

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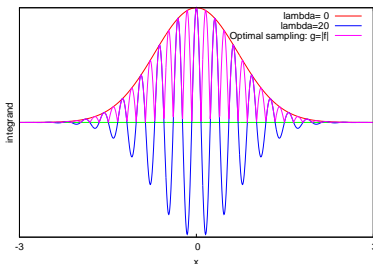
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- Optimal  $g$ ? Minimize relative fluctuations of denom.  $\rightarrow g(x) = |f(x)|$ ,  $\frac{f}{g} = \text{sign}(f)$

$$\langle W \rangle_f = \frac{\langle W \text{sign}(f) \rangle_{|f|}}{\langle \text{sign}(f) \rangle_{|f|}} \quad \text{"put sign in observable"}$$



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

Each meas. of  $\frac{f}{g}$  gives value  $\pm 1 \implies$  statistical error  $\approx \frac{1}{\sqrt{\# \text{ meas.}}}$

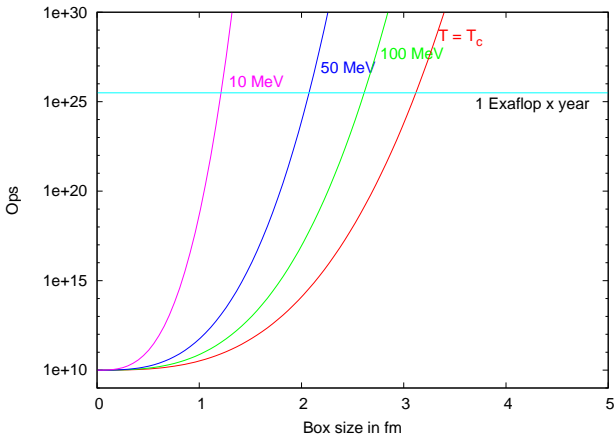
Constant relative accuracy  $\implies$  **need statistics  $\propto \exp(+2\frac{V}{T} \Delta f)$**

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

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

$\Delta f$



## Sampling for QCD at finite $\mu$

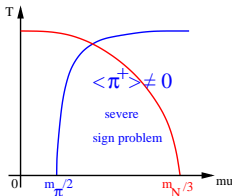
- QCD: sample with  $|\text{Re}(\det(\mu)^{N_f})|$  optimal, but not equiv. to Gaussian integral

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  $\pi^+$  when  $|\mu| > \mu_{\text{crit}}(T)$

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

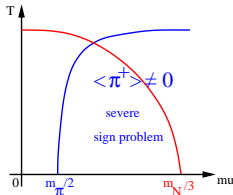


$\Delta f(\mu^2, T)$  large in the Bose phase  
 $\rightarrow$  “**severe**” sign pb.

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 $Z_{\text{QCD}} \leftrightarrow Z_{|\text{QCD}|}$  by changing fermion b.c.  $\Rightarrow$  ratio **UV-finite**

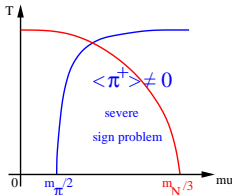
For  $T, \mu \ll m_p$ , **analytic** results via RMT/ $\chi$ PT

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For  $T, \mu \ll m_p$ , **analytic** results via RMT/ $\chi$ PT

Splittorff, Verbaarschot et al.

- Can improve by incorporating **baryons** via HRG  $\rightarrow$  Prediction: **1005.0539**

$\langle \text{sign} \rangle \gtrsim 0.1 \Leftrightarrow \mathcal{O}(10)$  baryons max. at  $T \lesssim T_c$  (less as  $T \searrow$ , hardly more as  $V \nearrow$ )

# Reweighting strategies

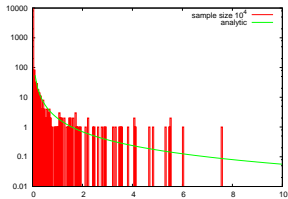
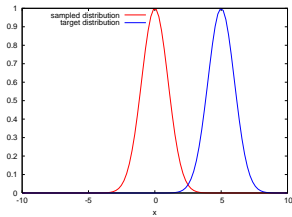
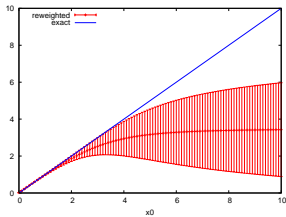
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- Sample  $\mu = 0$  ensemble? **worse**, because reweighting factor fluctuates **also in magnitude** → increased statistical errors
- Further danger: **“overlap pb.”** between sampled and reweighted ensembles → **WRONG** estimates in reweighted ensemble for finite statistics
- Example: sample  $\exp(-\frac{x^2}{2})$ , reweight to  $\exp(-\frac{(x-x_0)^2}{2})$  →  $\langle x \rangle = x_0$  ?



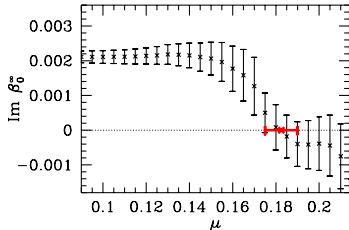
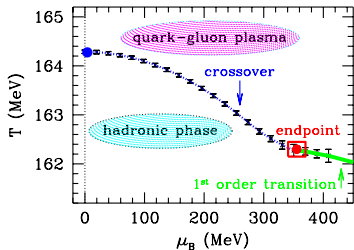
- Estimated  $\langle x \rangle$  saturates at largest sampled  $x$ -value
- Error estimate too small

Insufficient overlap ( $x_0 = 5$ )

Very non-Gaussian distribution of reweighting factor  
**Log-normal** Kaplan et al.

## Reweighting from $\mu = 0$ : multi-parameter

- Fodor & Katz: sample ( $\mu=0, \beta=\beta_c$ ) and reweight with  $\left(\frac{\det(\mu)}{\det(\mu=0)} \times e^{-\Delta\beta S_{YM}}\right)$  along pseudo-critical line  $T_c(\mu)$ 
  - fluctuations in reweighting factor compensate between det and  $S_{YM}$
  - improved (ensured?) overlap: both phases sampled



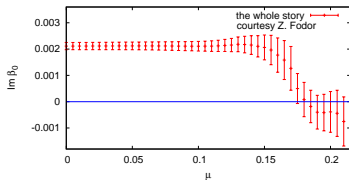
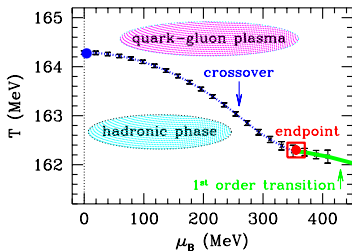
hep-lat/0402006 (physical quark masses,  $N_t=4$ )  $\rightarrow (\mu_E^q, T_E) = (120(13), 162(2))\text{MeV}$

- Abrupt qualitative change near  $\mu_E$ :



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abrupt change of physics or breakdown of reweighting ? (see later)

- Revival (fast det Wilson fermions): Ukawa et al., Nakamura et al.

# Change of strategy

Reweighting gives **exact answer in small volumes** (work  $\sim \exp(V)$ ) in principle

In practice: may fail without letting you know!

Try instead: **approximate answer in large volume** ?

And – perhaps – full confidence in results

Consider expansion parameter  $\frac{\mu}{T} \lesssim 1$ :

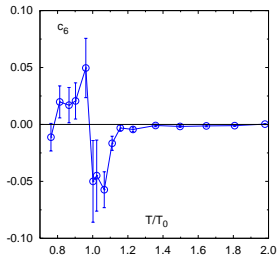
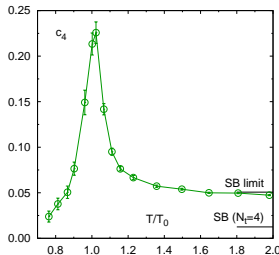
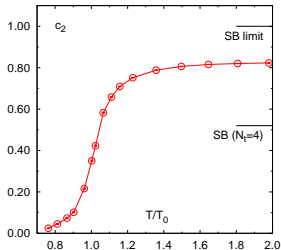
- Truncated **Taylor expansion** about  $\mu = 0$
- **Imaginary  $\mu$**  + polynomial fit + analytic continuation

$$P(T, \mu) = \underbrace{P(T, \mu = 0)}_{\text{indep. calc.}} + \Delta P(T, \mu),$$

$$\frac{\Delta P(T, \mu)}{T^4} = \sum_{k=1} c_{2k}(T) \left(\frac{\mu}{T}\right)^{2k}$$

$$c_{2k} = \langle \text{Tr}(\text{degree } 2k \text{ polynomial in } \mathcal{D}^{-1}, \frac{\partial \mathcal{D}}{\partial \mu}) \rangle_{\mu=0} \rightarrow \text{vanilla HMC}$$

- From  $\{c_{2k}\}$ , obtain **all thermodynamic info**: EOS *and*  $T_c(\mu)$  *and* crit. pt. *and* ...
- As  $\frac{\mu}{T}$  increases, need **higher-order  $c_{2k}$ 's** to control truncation error



## Taylor expansion: nitty-gritty

$$\begin{aligned}
 c_6 \rightarrow \frac{\partial^6 \ln \det M}{\partial \mu^6} &= \text{tr} \left( M^{-1} \frac{\partial^6 M}{\partial \mu^6} \right) - 6 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^5 M}{\partial \mu^5} \right) \\
 &- 15 \text{tr} \left( M^{-1} \frac{\partial^2 M}{\partial \mu^2} M^{-1} \frac{\partial^4 M}{\partial \mu^4} \right) - 10 \text{tr} \left( M^{-1} \frac{\partial^3 M}{\partial \mu^3} M^{-1} \frac{\partial^3 M}{\partial \mu^3} \right) \\
 &+ 30 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^4 M}{\partial \mu^4} \right) + 60 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^2 M}{\partial \mu^2} M^{-1} \frac{\partial^3 M}{\partial \mu^3} \right) \\
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 &- 120 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^3 M}{\partial \mu^3} \right) \\
 &- 180 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^2 M}{\partial \mu^2} M^{-1} \frac{\partial^2 M}{\partial \mu^2} \right) \\
 &- 90 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^2 M}{\partial \mu^2} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^2 M}{\partial \mu^2} \right) \\
 &+ 360 \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^2 M}{\partial \mu^2} \right) \\
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 \end{aligned}$$

Now estimate all Traces by sandwiching between noise vectors:

$$\text{Tr} \mathcal{O} = \langle \eta^\dagger \mathcal{O} \eta \rangle_\eta, \text{ where } \langle \eta_x^\dagger \eta_y \rangle = \delta_{xy} \rightarrow \text{GPU farm}$$

# Complexity of Taylor expansion approach?

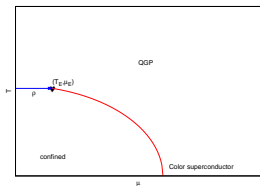
Effects of increasing Taylor order  $k$ :

- $c_{2k} = \langle \text{Tr}(\text{ degree } 2k \text{ polynomial in } \mathcal{D}^{-1}, \frac{\partial \mathcal{D}}{\partial \mu}) \rangle_{\mu=0}$  → nb. terms  $\sim 6^{2k}$
- **Cancellations:**  $c_{2k}$  finite as  $V \rightarrow \infty$ , but sum of terms, each possibly  $\sim V^{2k}$

ie. the sign problem fights back!

- $c_{2k}$  obtained as average over less and less Gaussian dist. → stat. error?
- $c_{2k} \sim 2k$ -point function → need larger volumes

Current best:  $N_t=6$ , **8th order** ( $c_2, c_4, c_6, c_8$ ) [Gavai & Gupta, 0806.2233](#)



Need *much* higher order

to estimate convergence radius → critical point

[Karsch, Schaefer et al, 1009.5211](#)

## Imaginary $\mu$ : similar but simpler – probably cheaper

- Simulate at several values of  $\mu = i\mu_I$ : **no sign pb.**
- Fit  $\langle \mathcal{O} \rangle(\mu_I) = \sum_k d_k \left(\frac{\mu_I}{T}\right)^k$ 
  - For pressure, take eg.  $\mathcal{O} = n_B = \frac{\partial P}{\partial \mu_B}$  and integrate fitted polynomial
  - Analytic continuation trivial:  $i\mu_I \rightarrow \mu$
  - **Stat. error** analysis simple: data at different  $\mu_I$ 's uncorrelated
  - **Systematic error**: order of truncation, fitting range

**No free lunch**: fit insensitive to  $d_k$  because  $\left(\frac{\mu_I}{T}\right)^k \ll 1$

**Advantage** over Taylor expansion: milder  $V$ -dependence?

- $\left|\frac{\mu_I}{T}\right| < \frac{\pi}{3}$ , **Roberge-Weiss** singularity  
Conformal mapping to unit disk

Morita et al., 1008.4549

## Other approaches

- **Canonical ensemble:**  $Z_Q = \int d(\frac{\mu}{T}) e^{i\frac{\mu}{T} Q} Z(\mu = i\mu_I)$

now with fast and accurate Fourier transform

Alford, Wilczek et al., PDF & Kratochvila, K.F. Liu et al., Nakamura, Wenger, ..

- **Density of states** a.k.a. histogram method:

$$Z(\mu) = \int dx \underbrace{\int \mathcal{D}U \delta(W(U) - x) \det(\mu) e^{-S_{YM}}}_{\rho(W;x)}$$

2d variant  $\rho(P, \left| \frac{\det(\mu)}{\det(0)} \right|)$  Ejiri et WHOT-QCD

Considerable technical progress but no breakthrough so far

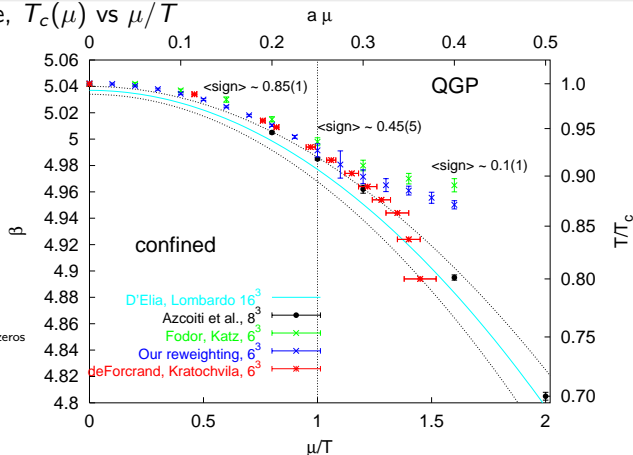
- **Complex Langevin?** progress: now *converges* to the right or wrong answer

Aarts, Seiler, Stamatescu

# Valuable crosschecks

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

Here,  $T_c(\mu)$  vs  $\mu/T$



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

imaginary  $\mu$   
 2 param. imag.  $\mu$   
 dble reweighting, LY zeros  
 Same, susceptibilities  
 canonical

More recent crosschecks (Wilson fermions):

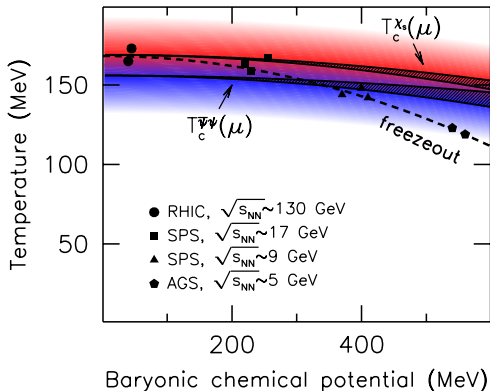
- Reweighting  $\leftrightarrow$  Taylor expansion
- Reweighting  $\leftrightarrow$  canonical

Nagata & Nakamura  
 Takeda, Kuramashi & Ukawa

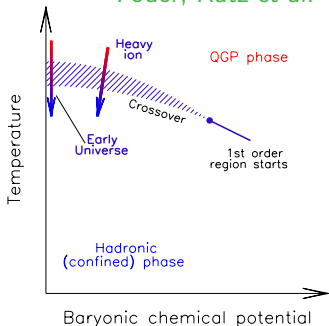


# State of the art

- **Curvature** of crossover  $T_c(\mu)$  in continuum limit (4 deriv. of  $P$ )



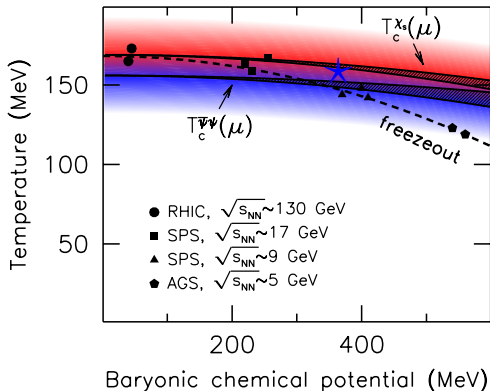
Fodor, Katz et al.



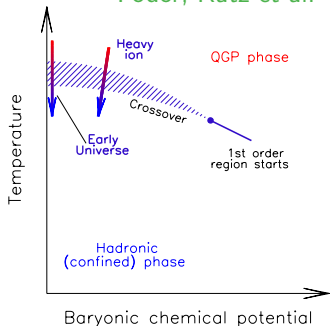
- $T_c(\mu)$  flatter than experimental heavy-ion freeze-out curve (different things)
- Different definitions of  $T_c(\mu)$  do not meet: no signal of critical point for  $\frac{\mu_q}{T} \lesssim \mathcal{O}(1)$

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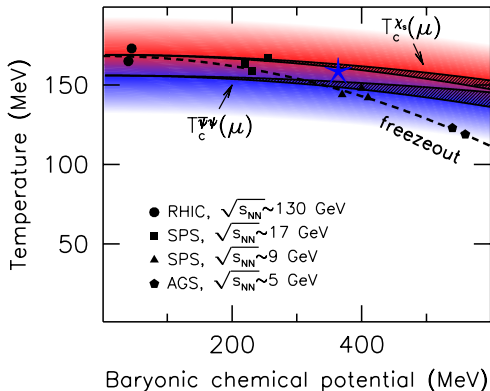
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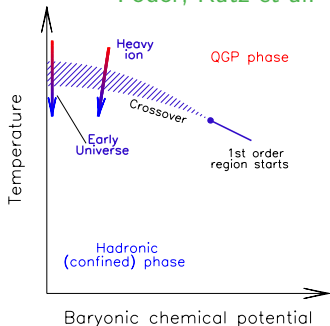
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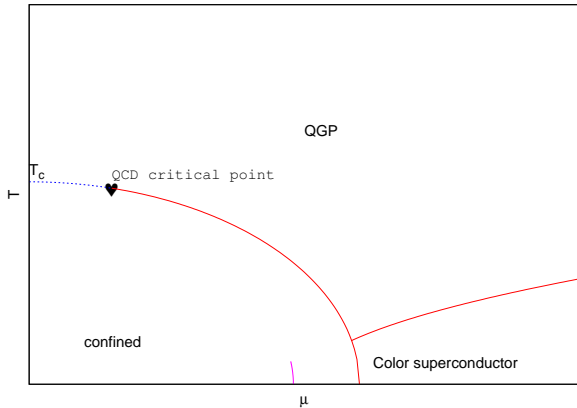
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- Next order (8 deriv. of  $P$ ) on coarse lattice: weakening of transition PdF & Philipsen

# Possible phase diagrams of QCD

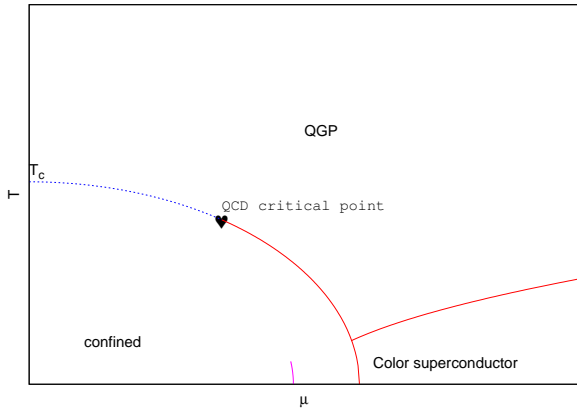
Where is the QCD critical point?



Exciting!

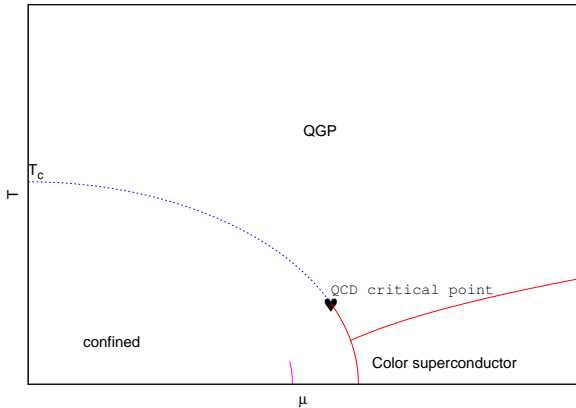
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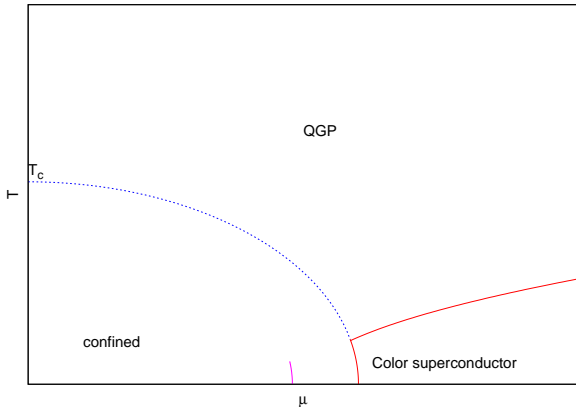
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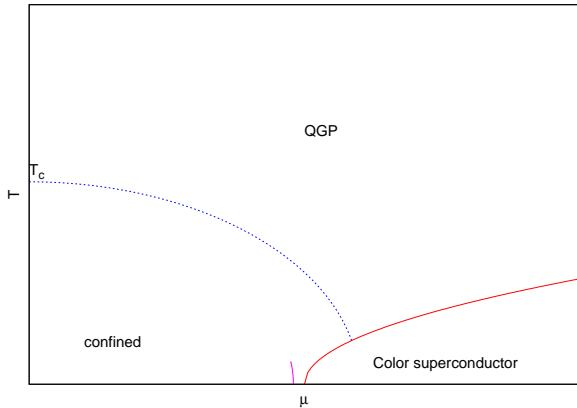
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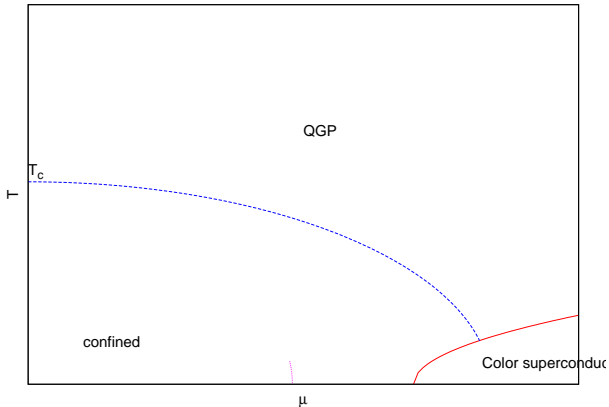
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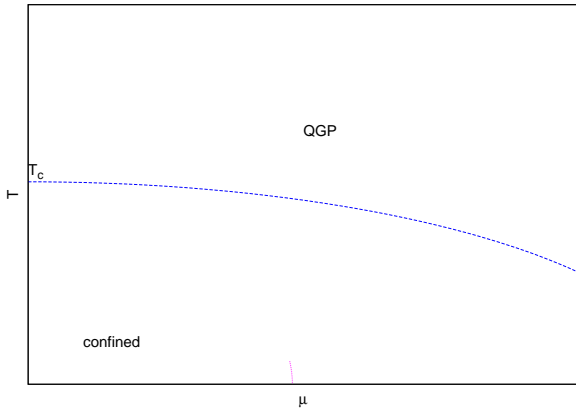
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# Possible phase diagrams of QCD

Where is the QCD critical point?



Boring but plausible!

Determining the QCD phase diagram remains just as important

cf. [Georges Charpak](#)

# How to make the sign problem milder?

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

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

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  $H$

QCD physical states are **color singlets**  $\rightarrow$  Monte Carlo on **colored** gluon links is bad idea

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:** so far, turn off **4-link coupling**  in  $\beta \sum_P \text{ReTr} U_P$  by setting  $\beta=0$

$\beta = 0$ : strong-coupling limit  $\longleftrightarrow$  continuum limit ( $\beta \rightarrow \infty$ )

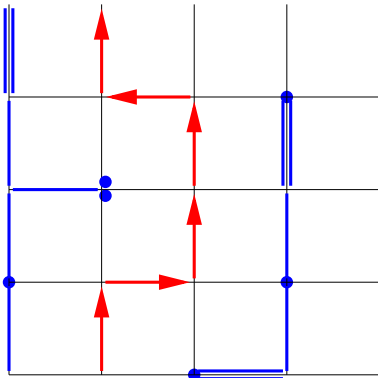


# Strong coupling limit at finite density

Chandrasekharan, Wenger, PdF, Ohnishi, ...

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

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

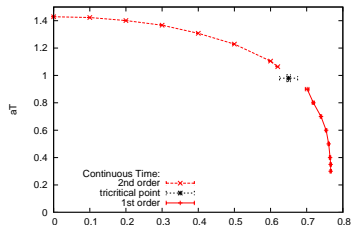


- Constraint at every site (Grassmann):  
3 meson symbols ( $\bullet$   $\bar{\psi}\psi$ , meson hop)  
or a baryon loop

Point-like, hard-core baryons in pion bath

- Sign pb.:  $\Delta f$  reduced by  $\mathcal{O}(10^4)$

→ full phase diagram

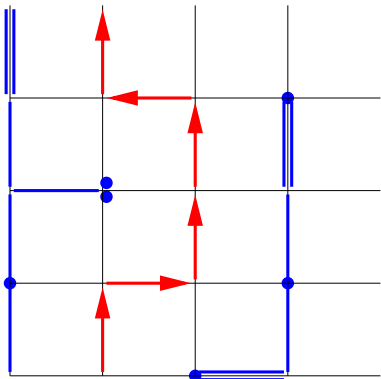


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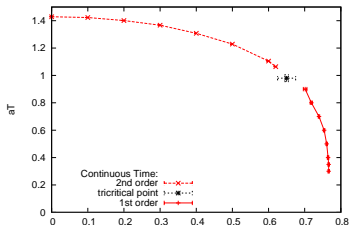
- Baryon: (point-like core + pion cloud)
- Nuclear potential: (hard-core + Yukawa)

- Constraint at every site (Grassmann):  
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Point-like, hard-core baryons in pion bath

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→ full phase diagram



# Conclusions

- Finite density LQCD suffers from **sign problem**:  $S/N \sim \exp(-\#\text{d.o.f.})$

→ only small  $V$ , small  $\mu/T$

- Simulations still at an early, “experimental” stage
- No reliable indication of QCD critical point [yet]
- **Progress**: - **analytic understanding** of severity of sign problem  
- new direction: reverse order of integration (quarks  $\leftrightarrow$  gluons)

Finite density QCD is important enough to keep trying

Hardware improvement alone will not suffice



A true challenge (= **opportunity**) for computational physicists!

# Backup: complex Langevin 80's revival Aarts, Seiler, Stamatescu, Berges,..

- Real action  $S$ : Langevin evolution in Monte-Carlo time  $\tau$  Parisi-Wu

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

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:

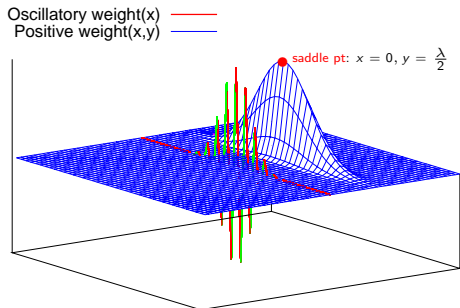
$$Z(\lambda) = \int dx \exp(-x^2 + i\lambda x)$$

Complexify:

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

For any observable  $W$ ,

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





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

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

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

- Mitigated with variational baryon ops.  $\rightarrow m_{\text{eff}}$  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
- Binding energy of  $^3\text{He}$ , He Kuramashi, Ukawa et al., 0912.1383

Here, we want a finite baryon density  $\rightarrow N \propto V$ , ie. chem. pot.  $\mu \neq 0$