# The sign problem in lattice QCD at finite density

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QISM, Innsbruck, Sept. 2012

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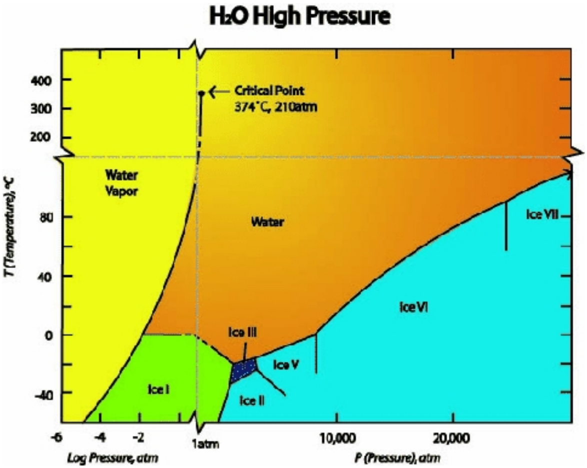
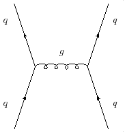
Water changes its state when heated or compressed




What happens to quarks and gluons when heated or compressed?

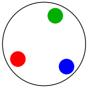
# Quantum Chromodynamics: confinement under normal conditions

- Quarks and gluons carry a *color* charge
- Quarks interact by exchanging gluons

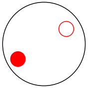



- Quarks are confined into color-neutral (color singlet) bound-states (hadrons):

$qqq$ baryons: proton, neutron, ...

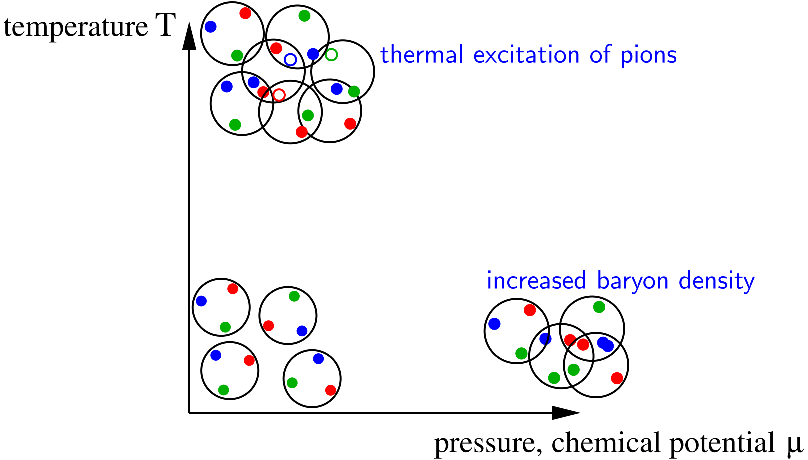


$q\bar{q}$ mesons: pion (lightest), kaon, rho, ...



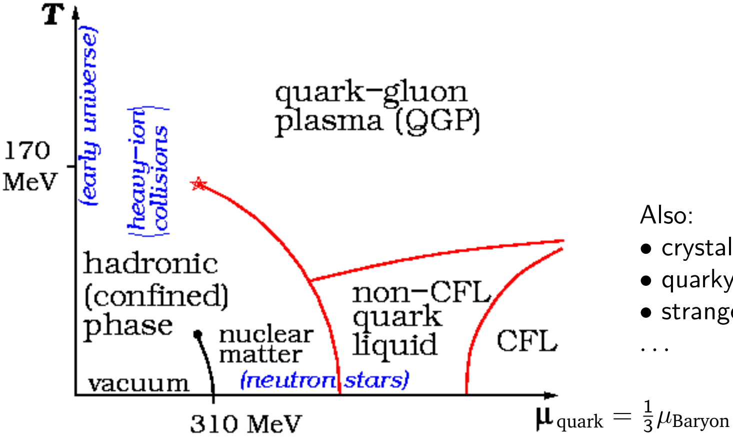
# QCD under extreme conditions

Compress or heat baryons: hadrons overlap $\rightarrow$ confinement "lost"
$\Rightarrow$ expect interesting/unusual behaviour



# The phase diagram of QCD according to Wikipedia

Current conjecture



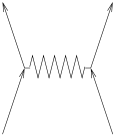

Also:

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

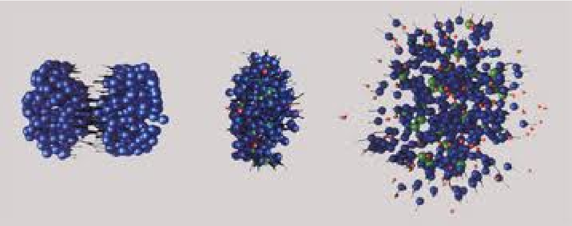
A vast world to explore!

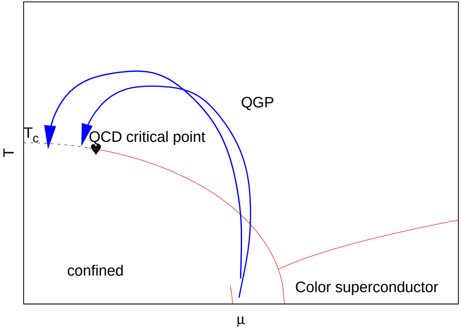
QCD critical point: a challenge for experiment and theory

# Probing the QCD phase diagram

- Experiment: heavy-ion collisions
- Theory:
  - Effective models:  $\Longrightarrow$  systematic error?
  - Lattice QCD

# Heavy-ion collisions I





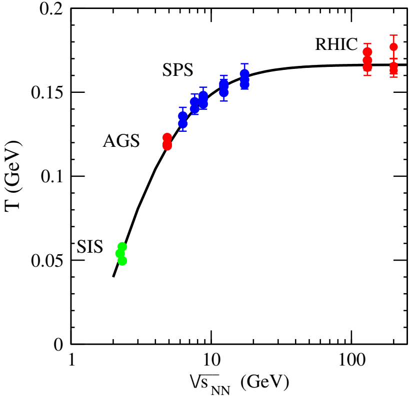

Knobs to turn:
- atomic number of ions
- collision energy $\sqrt{s}$

# Heavy-ion collisions II

Extract $T$ and $\mu$ from measured abundances of various hadrons

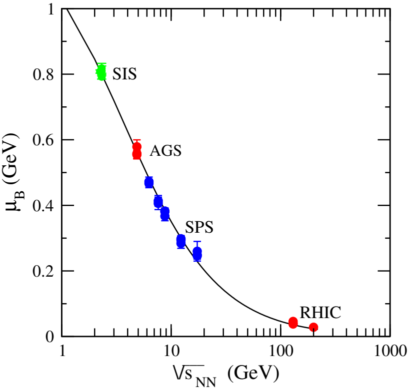
Cleymans et al.

*Freeze-out* temperature




As $\sqrt{s}$ increases: $T$ increases

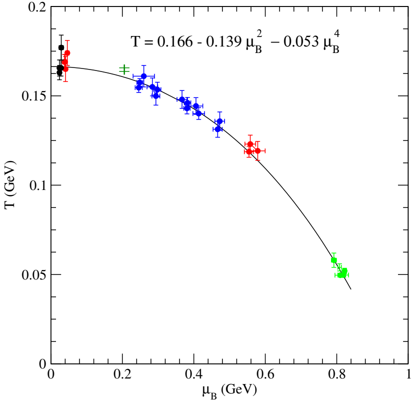
*Freeze-out* chemical potential

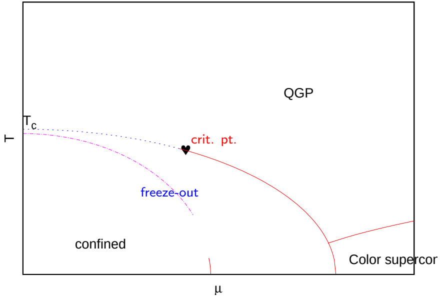



Net excess of matter constant
$\rightarrow$ baryon *density* (and $\mu$) decreases

# Heavy-ion collisions III

Freeze-out curve: quarks have finished recombining into hadrons → $T_{\mathrm{freeze-out}} \leq T_c$

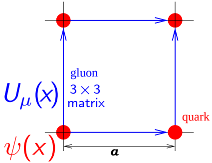


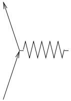
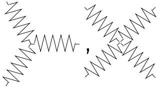
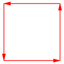

- RHIC, LHC: passage through strongly interacting quark-gluon plasma at $T \gtrsim 170$ MeV
- So far, no sign of QCD critical point (esp. RHIC beam energy scan)
- Difficulty I: high density with low temperature (↔ LHC)
- Difficulty II: signature of critical point may be washed out before freeze-out

# Lattice QCD

space + imag. time → 4*d* 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 $\bar{\psi}\not{D}\,\psi$
  -  $\longrightarrow$ $\beta\ \mathrm{ReTr}\,U_P$, $U_P$ 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) → determinant ($N_f = 2 \to$ squared)

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

# Sampling the determinant

- Gaussian integrals:

$$\int \mathcal{D}\bar{\psi}_1 \mathcal{D}\psi_1 \mathcal{D}\bar{\psi}_2 \mathcal{D}\psi_2 \; e^{-[\bar{\psi}_1 \not{D}\, \psi_1 + \bar{\psi}_2 \not{D}\, \psi_2]} = \det{}^2 \not{D} \; = \int \mathcal{D}\phi^* \mathcal{D}\phi \; e^{-\phi^\dagger \frac{1}{\not{D}^\dagger \not{D}} \phi}$$

- Computation of det $\not{D}$ not needed: sample $\phi$ instead

- Works provided det $\not{D}$ real

# Lattice QCD Monte Carlo: sources of errors

- Systematic errors:

  $L \to \infty$, thermodynamic limit

  $a \to 0$, continuum limit

  $m_q \searrow m_{\text{phys}}$

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

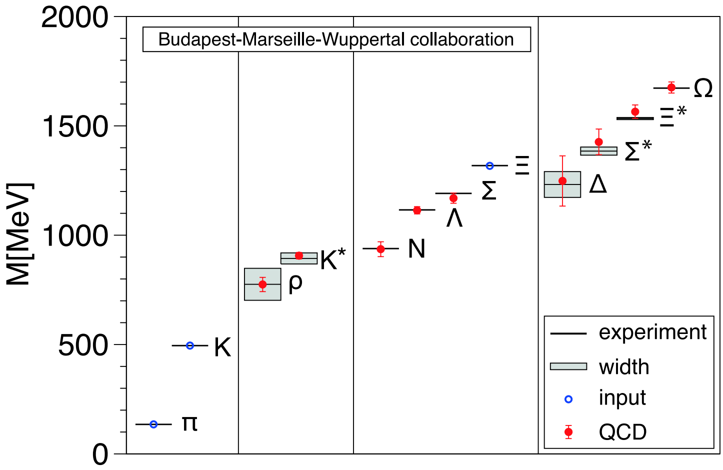
- Statistical (Monte Carlo) errors: $\propto 1/\sqrt{\#\text{configs.}}$

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

# Lattice QCD Monte Carlo: high precision hadron masses



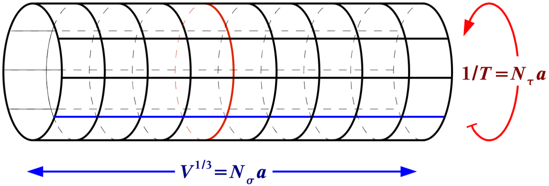

Z. Fodor et al., Science 2008

- Input: $m_\pi, m_K, m_\Xi \;\rightarrow\; a, m_{u,d}, m_s$
- Output: all groundstate masses with $\sim 3\%$ accuracy

# QCD thermodynamics on the lattice: modify boundary conditions

- Finite $T$:

$$Z = \mathrm{Tr}\ e^{-\frac{1}{T}H}$$




- Finite $\mu$: $U_4(x) \to e^{+a\mu} U_4(x)$, $U_{-4}(x) \to e^{-a\mu} U_{-4}(x)$ in $S_E$

loops winding $k$ times around imaginary time direction multiplied by $\exp(k\frac{\mu}{T})$

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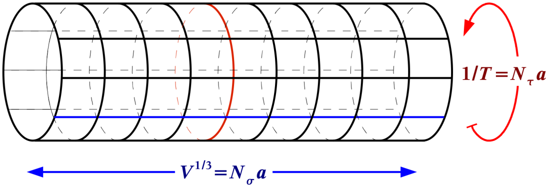


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$\mu > 0$ breaks charge-conjugation ($\approx$ complex conj.) symmetry $\Rightarrow \det \not{D}(\mu)$ complex

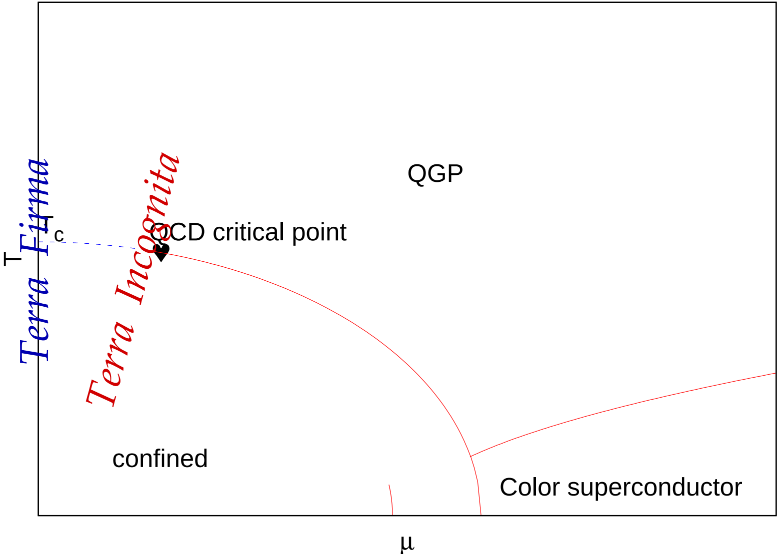
Formally: $\gamma_5$-hermiticity $\qquad \det \not{D}(\mu) = \det^* \not{D}(-\mu^*)$

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

$$\Downarrow$$

$\mu \neq 0$: no probabilistic interpretation of $\det \not{D} \in C$, ie. sign problem

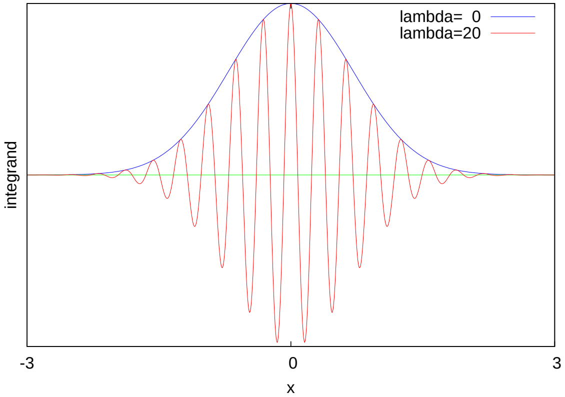
# Sign pb: long-standing roadblock to progress




"Sign 2012", Regensburg → 50 ways to leave your lover

# Complex actions: sampling oscillatory integrands

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




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

$\rightarrow$ truncating deep in the tail at $x \sim \lambda$ gives $\mathcal{O}(100\%)$ error

"Every $x$ is important" $\leftrightarrow$ How to sample?

# Reweighting

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

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

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

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- In general: sample with $g(x) \geq 0 \rightarrow \langle W \rangle_f = \frac{\langle W \frac{f}{g} \rangle_g}{\langle \frac{f}{g} \rangle_g}$, $\frac{f}{g}$ is "reweighting factor"

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

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

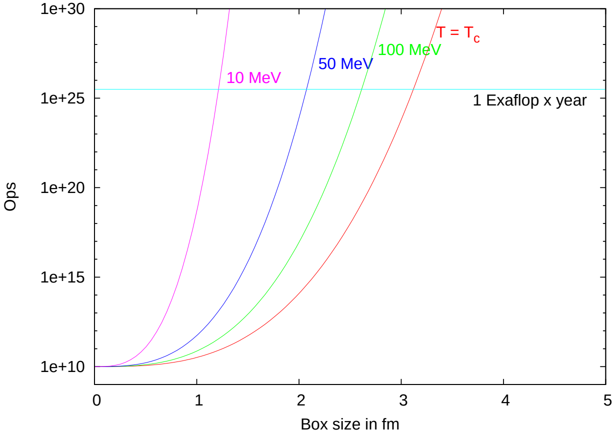
  Constant relative accuracy $\Longrightarrow$ $\boxed{\text{need statistics} \propto \exp(+2\frac{V}{T}\Delta f)}$

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

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

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

# Sampling for QCD at finite $\mu$

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

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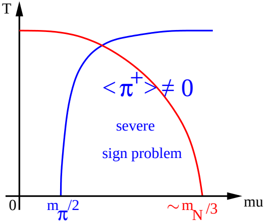
  couples to charged pions $u\bar{d} = \pi^+ \Rightarrow$ Bose condensation of $\pi^+$ when $|\mu| > \mu_{\mathrm{crit}}(T)$




$$\langle e^{i\mathrm{phase}} \rangle = \frac{Z_{\mathrm{QCD}}(\mu)}{Z_{|\mathrm{QCD}|}(\mu)} = e^{-\frac{V}{T}[f(+\mu,+\mu) - f(+\mu,-\mu)]}$$

$\Delta f(\mu^2, T)$ large in the Bose condensed phase

$\rightarrow$ "severe" sign pb. (esp. "Silver Blaze")

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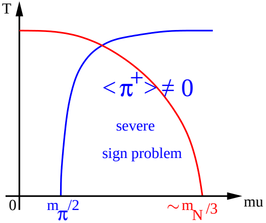


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- In region of *mild* sign pb., can estimate $\Delta f(\mu^2, T)$ analytically:

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

  Can use RMT/$\chi$PT (pions only) — Splittorff, Verbaarschot et al.

  Can use HRG (baryons included) — PdF, 1005.0539

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

# Reweighting strategies: Charybdis and Scylla

- Sample phase-quenched ensemble + reweight with $e^{i\theta} \to$ only 0711.0023, 1111.6363

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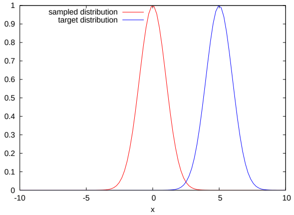
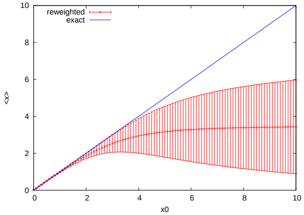
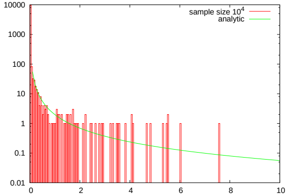
- Sample with $\det(\mu=0)$ ? worse, because reweighting factor $\frac{\det(\mu)}{\det(\mu=0)}$ fluctuates also in magnitude → increased statistical errors
- Further danger: "overlap problem" between sampled and reweighted ensembles → WRONG estimates in reweighted ensemble for finite statistics
- Example: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




Insufficient overlap ($x_0=5$)




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

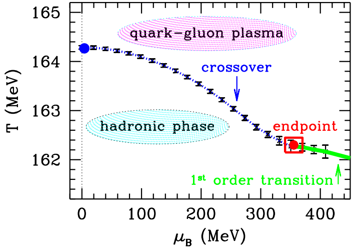


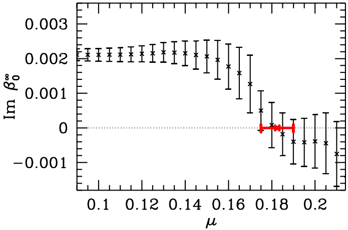

Very non-Gaussian distribution of reweighting factor

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, $N_t = 4$) $\rightarrow$ $(\mu_E^q, T_E) = (120(13), 162(2))$MeV

- Abrupt qualitative change near $\mu_E$:

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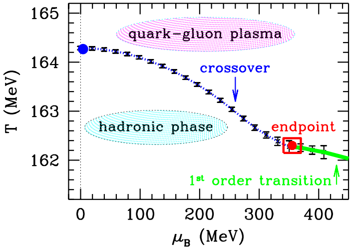


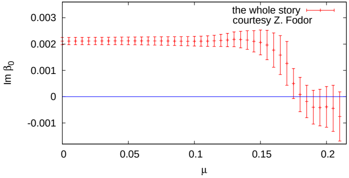


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abrupt change of physics or breakdown of reweighting ?

# 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 (no sign pb)

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

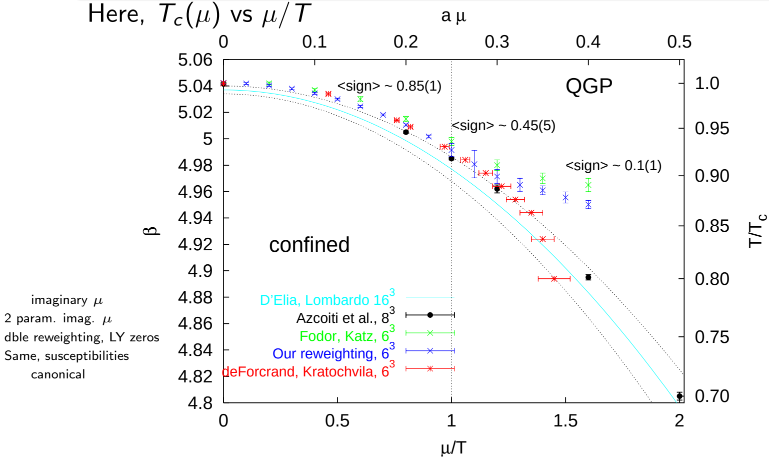
- Truncated Taylor expansion about $\mu = 0$
- Imaginary $\mu$ + polynomial fit + analytic continuation

Also "Voodoo approach": complex Langevin...

# 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

More recent crosschecks (Wilson fermions):

- Reweighting ↔ Taylor expansion — Nagata & Nakamura
- Reweighting ↔ canonical — Takeda, Kuramashi & Ukawa

# $\mu/T \gtrsim \mathcal{O}(1)$: how to make the sign problem milder?

- Severity of sign pb. is representation dependent:

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

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

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

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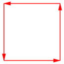
Usual:
- integrate over quarks analytically $\rightarrow \det(\{U\})$
- Monte Carlo over gluon fields $\{U\}$

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

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

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

# 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 degrees of freedom: meson & baryon worldlines

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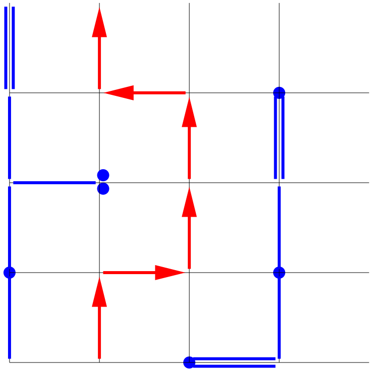

Constraint at every site:
3 blue symbols (• $\bar{\psi}\psi$, meson hop)
or a baryon loop

Update with worm algorithm

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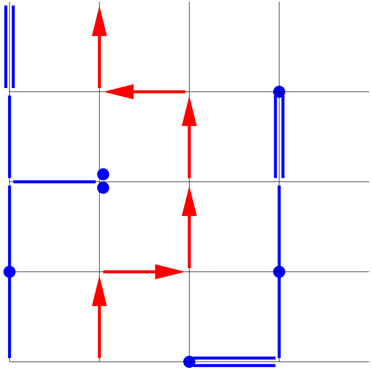

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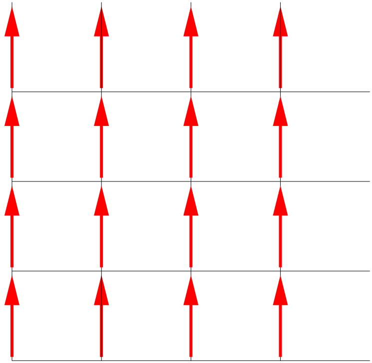
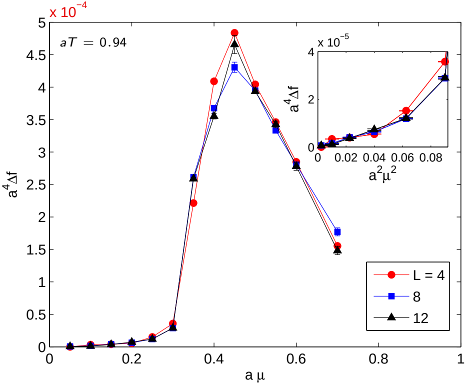


The dense (crystalline) phase:
1 baryon per site; no space left
$\rightarrow \quad \langle \bar{\psi}\psi \rangle = 0$

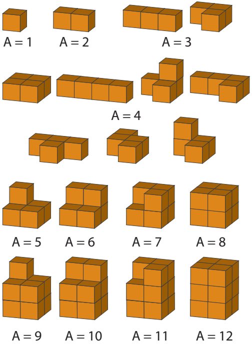
Update with worm algorithm

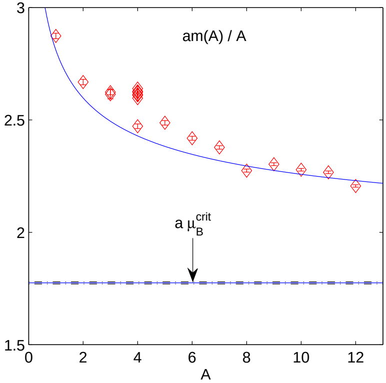
# Sign problem? Monitor $-\frac{1}{V}\log\langle\text{sign}\rangle$




- $\langle\text{sign}\rangle = \frac{Z}{Z_{||}} \sim \exp(-\frac{V}{T}\Delta f(\mu^2))$ as expected; $\Delta f \sim \mu^2 + \mathcal{O}(\mu^4)$
- Determinant method $\to \Delta f \sim \mathcal{O}(1)$. **Gain $\mathcal{O}(10^4)$ in the exponent!**
  - heuristic argument correct: color singlets closer to eigenbasis
  - negative sign caused by spatial baryon hopping:
    - no baryon $\to$ no sign pb (no silver blaze pb.)
    - saturated with baryons $\to$ no sign pb

# Results – Crude nuclear matter: spectroscopy

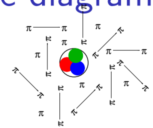


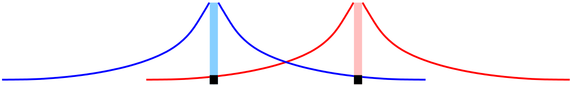

- Can compare masses of differently shaped "isotopes"
- $am(A) \sim a\mu_B^{\rm crit} A + (36\pi)^{1/3}\sigma a^2 A^{2/3}$, ie. (bulk + surface tension)

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

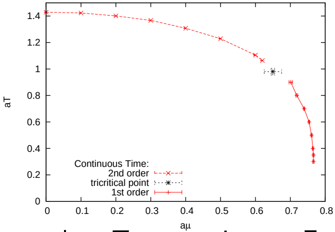
# Results II – Nuclear interactions and Phase diagram



- Baryon: point-like core (self-avoiding loop) disturbs pion bath
  $\Rightarrow$ macroscopic pion cloud $\Delta E_\pi(R) \propto \frac{\exp(-\mathbf{m}_{\rho/\omega} R)}{R} \times (-1)^{x+y+z}$
- Nuclear interaction from nucleon's core disturbing other nucleon's pion cloud
  Linear response $\Rightarrow$ $V_{NN}(R) \approx -2 \times \Delta E_\pi(R)$, ie. Yukawa!



- Phase diagram for $m_q = 0$: chiral transition line, with tricritical point




- Discretization error, esp. at low $T \to$ continuous Euclidean time Unger
- Latest news (arXiv:1208.2148):
  chiral symmetry restored at $T = 0$ for $N_f \geq 13 \to$ conformal phase

# Conclusions

- Sign problem frequent roadblock (fermions and/or bosons):
  $$S/N \sim \exp(-\#\text{d.o.f.})$$
- Hard pb, but technical (representation-dependent), not fundamental
- "Solving" (ie. eliminating) sign pb not necessary:
  just make it mild enough to reach desired $(V, \mu/T)$
- Different strategies (esp. change of variables) for different theories
- Useful guiding principle: work in approximate eigenbasis
- Lattice QCD: reverse usual order of integration (quarks $\leftrightarrow$ gluons)
- Strong coupling limit of Lattice QCD:
  - full numerical solution available (also for continuous Eucl. time)
  - interesting physics (toy model for nuclear matter)
  - no plaquette term $\rightarrow$ easier for quantum simulation
  - plaquette term can be induced eg. by additional heavy fermions